Introduction to Computational Physics

PHYS 250 (Autumn 2018) – Lecture 3

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Outline

1. *The physics of randomness and emergent properties*
   - Coin flips
   - Random walks
   - Central limit theorem and analytic descriptions of random behavior

Coin flips

See Sethna's text for more info

We began discussing random numbers last lecture. Let's continue on that topic and extrapolate to much deeper properties of physics.

Consider flipping a coin and recording the difference s_N between the number of heads and tails found. Each flip contributes $\ell_i = \pm 1$ to the total.
How big a sum

$$s_N = \sum_{i=1}^{N} \ell_i = (\text{heads} - \text{tails}) \tag{1}$$

do you **expect** after N flips? To answer the question regarding **expectations**, we need to be able to repeat the measurement many times and compute some statistics about what is going on.

Expectation values and statistics

The average of s_N is not a good measure for the sum, because it is zero (positive and negative steps equally likely). We could measure the average absolute value $\langle |s_N| \rangle$, but the root-mean-square (RMS) of the sum is better, $\sqrt{\langle s_N^2 \rangle}$. After each flip, the mean square is:

$$\begin{aligned}
\langle s_1^2 \rangle &= 0.5(-1)^2 + 0.5(1)^2 = 1 && (2)\\
\langle s_2^2 \rangle &= 0.25(-2)^2 + 0.5(0)^2 + 0.25(2)^2 = 2 && (3)\\
&\vdots && (4)\\
\langle s_N^2 \rangle &= \langle (s_{N-1} + \ell_N)^2 \rangle = \langle s_{N-1}^2 \rangle + 2\langle s_{N-1}\ell_N \rangle + \langle \ell_N^2 \rangle && (5)
\end{aligned}$$

Since $\ell_N = \pm 1$, middle term cancels (equal probability of ± 1) and thus

$$\begin{aligned}
\langle s_N^2 \rangle &= \langle s_{N-1}^2 \rangle + \langle \ell_N^2 \rangle = N - 1 + 1 && (6)\\
&= N && (7)\\
\sigma_s = \sqrt{\langle s_N^2 \rangle} &= \sqrt{N} && (8)
\end{aligned}$$

Scale invariance and universality

The discussion above highlights an important point that we will revisit in the case of random "motion", or random walks: **scale invariance and universality**.

- The rate of random $+1$'s and -1's look no different when viewed a "few" at a time, or hundreds at a time
- On scales where the individual coin tosses are not observable, you cannot pick out any "preferred" features

To put this in slightly more concrete terms that will be best studied with random walks

- **Scale invariance:** the fluctuations of the system occur at all length scales.
- **Universality:** the behavior of the system is independent of the microscopic details of that system

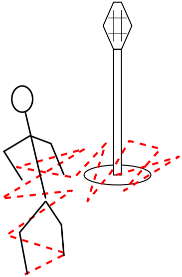
The latter is also deeply related to the **central limit theorem**.

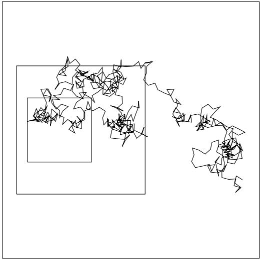
Random walks

Random walks also arise as trajectories that undergo successive random collisions or turns; for example, the trajectory of a perfume molecule in a sample of air.

We will study this example using N fixed length steps:

- ℓ_N: sequence of N steps
- L: length of each step
- $\vec{\ell}_i$: step of length L in the i direction
- d: number of dimensions
- Assume exactly uncorrelated, random steps in each dimension d





How long of a walk?

This lack of correlation says that the average dot product between any two steps ℓ_m and ℓ_n is zero

$$\langle \vec{\ell}_m \cdot \vec{\ell}_n \rangle = L \langle \cos\theta \rangle = 0 \tag{9}$$

where θ is the angle between the two steps. This implies that the dot product of $\vec{\ell}_N$ with $\vec{s}_{N-1} = \sum_{m=1}^{N-1} \vec{\ell}_m$ is zero. Again, we can work by induction:

$$\begin{aligned}
\langle \vec{s}_N^{\,2} \rangle &= \langle (\vec{s}_{N-1} + \vec{\ell}_N)^2 \rangle && (10)\\
&= \langle \vec{s}_{N-1}^{\,2} \rangle + \langle \vec{\ell}_N^{\ 2} \rangle && (11)\\
&= \langle \vec{s}_{N-1}^{\,2} \rangle + L^2 && (12)\\
&= NL^2 && (13)\\
\sigma_s = \sqrt{\langle s_N^2 \rangle} &= \sqrt{N}L && (14)
\end{aligned}$$

so the RMS distance moved is $\sqrt{N}L$.

Markov Chain Monte Carlo

A random walker is a specific subclass of a more general class of algorithms called **Markov chain Monte Carlo (MCMC)**.

A stochastic model describing a sequence of possible events in which the probability of each event depends only on the state attained in the previous event.

Some characteristics that distinguish this class of algorithms are:

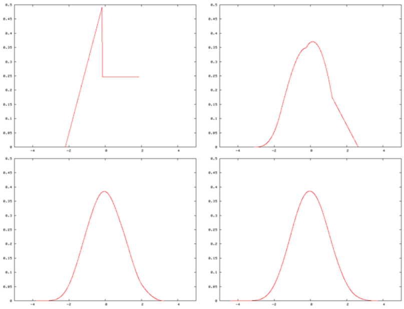
- Sequence of elements chosen from a fixed set using a probabilistic rule
- Chain is constructed by adding the elements sequentially
- Given the most recently added element, next element only depends on most recent addition

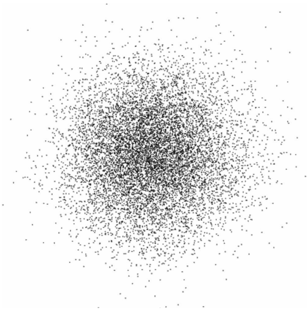
In the case of the random walker, the walker's position after N steps depends on the sequence of steps in the past, and cannot be predicted. However, a pattern emerges for an **ensemble** of positions after many such walks.

Central limit theorem

You're all likely familiar with the central limit theorem:

When independent random variables are added, their properly normalized sum tends toward a normal distribution, even if the original variables themselves are not normally distributed.





The picture on the right shows the end points of many separate random walks.

Diffusion equation

In cases in which simple behavior seemingly emerges from an ensemble of irregular, jagged random walks (in the continuum limit of long length and time scales) their evolution can be described by the diffusion equation:

$$\frac{\partial \rho}{\partial t} = D\nabla^2 \rho = D\frac{\partial^2 \rho}{\partial x^2} \tag{15}$$

The diffusion equation can describe the evolving density $\rho(x, t)$ of a local cloud of perfume as the molecules **random walk** through collisions with the air molecules. Alternatively, it can describe the probability density of an individual particle as it **random walks** through space; if the particles are non-interacting, the probability distribution of one particle describes the density of all particles.

Random diffusion (I)

Consider a general, uncorrelated random walk where at each time step Δt the particle's position x changes by a step ℓ:

$$x(t + \Delta t) = x(t) + \ell(t). \tag{16}$$

Let the probability distribution for each step be $\chi(\ell)$, which in our case is a discrete probability (e.g. for the 2D random walk, $\chi(\ell) = \delta(|\ell| - L)$ with equal probability in $\pm x, \pm y$). We will assume that χ has mean zero and standard deviation a. The first few moments of χ are therefore:

$$\int \chi(z)dz = 1 \tag{17}$$

$$\int z\chi(z)dz = 0 \tag{18}$$

$$\int z^2\chi(z)dz = a^2 \tag{19}$$

Random diffusion (II)

For the particle to go from x' at time t to x at time $t+\Delta t$, the step $\ell(t)$ must be $x - x'$. This happens with probability $\chi(x-x')$ times the probability density $\rho(x', t)$ that it started at x'. Integrating over original positions x', we have:

$$\begin{aligned}\rho(x, t+\Delta t) &= \int_{-\infty}^{+\infty} \rho(x', t)\chi(x-x')dx' && (20)\\ &= \int_{-\infty}^{+\infty} \rho(x-z, t)\chi(z)dz && (21)\end{aligned}$$

where we have changed variables $x' \to z = x - x'$. Now, perform a Taylor expansion in z:

$$\begin{aligned}\rho(x, t+\Delta t) &\approx \rho(x,t) + \frac{1}{2}\frac{\partial^2 \rho}{\partial x^2}\int z^2 \chi(z)dz && (22)\\ &\approx \rho(x,t) + \frac{a^2}{2}\frac{\partial^2 \rho}{\partial x^2} && (23)\end{aligned}$$

Slow random diffusion

If the diffusion is also slow, such that the time derivative of ρ is approximately linear with respect to time and $\rho(x, t + \Delta t) - \rho(x, t) \approx (\frac{\partial \rho}{\partial t})\Delta t$, then

$$\frac{\partial \rho}{\partial t} = \frac{a^2}{2\Delta t}\frac{\partial^2 \rho}{\partial x^2}. \tag{24}$$

This is the diffusion equation Eq. 15 with $D = \frac{a^2}{2\Delta t}$.

The point is that we obtained an analytical description of a random walk via the diffusion equation under minimal assumptions: the probability distribution is broad and slowly varying compared to the size and time of the individual steps.